

Resonant x-ray Raman scattering spectra of Cu *dd* excitations in $\text{Sr}_2\text{CuO}_2\text{Cl}_2$

J.-H. Guo, P. Kuiper, C. S  the, and J. Nordgren

Department of Physics, Uppsala University, Box 530, 751 21 Uppsala, Sweden

The energies of the lowest excitations in the Cu-based superconductors are basic quantities of interest in the ongoing struggle to determine the underlying electronic structure and elementary excitations. The energies of the local on-site *dd* excitations have been a topic debate recently.

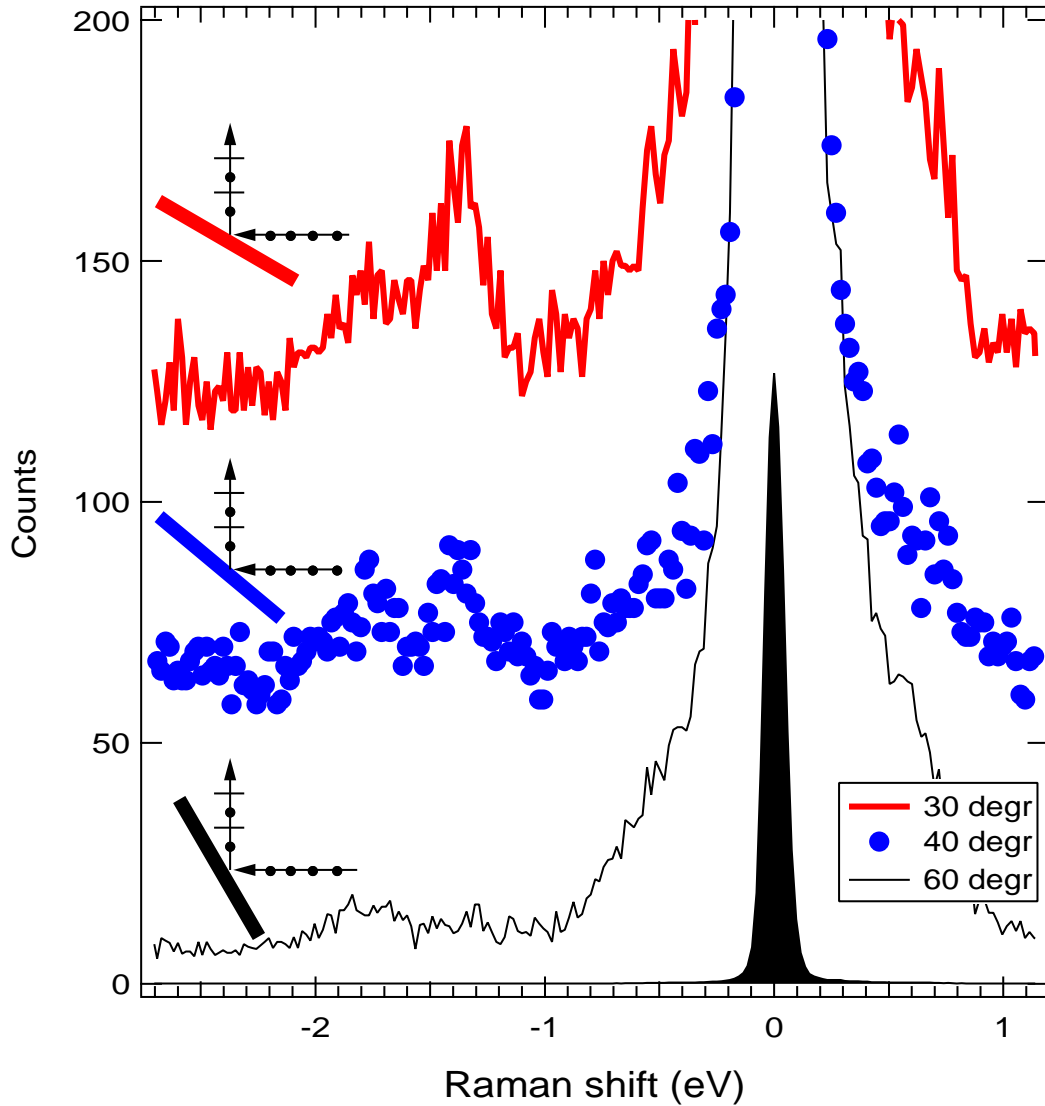


FIG. 1. Polarization-dependent x-ray resonant Raman spectra at the Cu M_3 resonance (74 eV). The angle between the emission direction and the sample normal is 30°, 40°, and 60°, from top to bottom. The last spectrum is also shown reduced by a factor of 200.

Resonant x-ray Raman spectroscopy (RXRS) has the makings of a powerful technique to study the elementary excitations in solids. Using excitation energies at specific core-level thresholds one can identify the excitations, determine their atomic origin, and, as shown by choosing core level with strong spin orbit coupling, one can also observe the local spin flip excitations whose energies are determined by exchange and superexchange interactions with neighboring spins [1]. Only recently has the resolution of RXRS become sufficiently high to study valence-valence excitations. Molecules and wide-band solids have attracted considerable interest [2], but the method has also been used to study charge-transfer excitations in correlated systems [3] and dd -excitations in MnO [4].

We present resonant x-ray Raman scattering results on $\text{Sr}_2\text{CuO}_2\text{Cl}_2$, a model compound for high- T_c superconductors [5]. The experiment was performed at beamline 7 of the Advanced Light Source (ALS) at Berkeley. The dd excitations can be observed and show that the polarization dependence can be used to identify the dd excitations. We find the transition from the $d_{x^2-y^2}$ ground state to the d_{xy} excited state at 1.35 eV and to the degenerated d_{xz} and d_{yz} excited states at 1.7 eV. From analysis of the polarization dependence we conclude that the $d_{3z^2-r^2}$ orbital energy is at 1.5 eV and not in the mid infrared (0.5 eV) as recently suggested. We use recent theoretical arguments to show that the $d_{3z^2-r^2}$ excitation is accompanied by a local spin flip resulting in a shift upwards of 0.2 eV due to the exchange interaction with neighboring spins.

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Principal investigator: E. Joseph Nordgren, Department of Physics, Uppsala University. E-mail: joseph@fysik.uu.se. Telephone: +46 18 4713554.